



PERGAMON

Computers & Chemical Engineering

An International Journal
of Computer Applications in
Chemical Engineering

List of Contents and Author Index
Volume 19, 1995

Computers & Chemical Engineering

An International Journal of
Computer Applications in
Chemical Engineering

Editor

G. V. Reklaitis, *School of Chemical Engineering, CHME Building 1283, Purdue University, West Lafayette, IN 47907, U.S.A.*

Associate Editors

M. Morari, *Institut für Automatik, ETH-Z/ETL 129, CH-8092, Zurich, Switzerland*

J. W. Ponton, *Department of Chemical Engineering, University of Edinburgh, King's Building, Mayfield Road, Edinburgh EH9 3JL, U.K.*

Editorial Advisory Board

G. Buzzi-Ferraris <i>Milan, Italy</i>	I. E. Grossmann <i>Pittsburgh, Pennsylvania</i>	L. C. Puigjaner <i>Barcelona, Spain</i>	G. Stephanopoulos <i>Cambridge, Massachusetts</i>
B. Carnahan <i>Ann Arbor, Michigan</i>	I. Hashimoto <i>Kyoto, Japan</i>	E. M. Rosen <i>St Louis, Missouri</i>	W. E. Stewart <i>Madison, Wisconsin</i>
J. Cerdá <i>Santa Fe, Argentina</i>	T. Hertzberg <i>Trondheim, Norway</i>	R. W. H. Sargent <i>London, England</i>	T. Umeda <i>Chiba, Japan</i>
B.-z. Chen <i>Beijing, China</i>	M. Kubíček <i>Prague, Czech Republic</i>	J. D. Seader <i>Salt Lake City, Utah</i>	A. W. Westerberg <i>Pittsburgh, Pennsylvania</i>
D. Depeyre <i>Chatenay-Malabry, France</i>	M. L. Michelsen <i>Lyngby, Denmark</i>	W. D. Seider <i>Philadelphia, Pennsylvania</i>	J. D. Wright <i>Pointe-Claire, Canada</i>
T. F. Edgar <i>Austin, Texas</i>	R. L. Motard <i>St Louis, Missouri</i>	J. H. Seinfeld <i>Pasadena, California</i>	D. Edelson <i>Tallahassee, Florida</i>
L. B. Evans <i>Cambridge, Massachusetts</i>	R. G. H. Prince <i>Sydney, Australia</i>	M. Shacham <i>Beer Sheva, Israel</i>	Liaison Member <i>Computers & Chemistry</i>

Publishing Office

(Production Editor: T. Beuzeval)

Elsevier Science Ltd, The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, U.K.

[Tel. Oxford (01865) 843000; Fax 843969]

Subscription and Advertising Offices

North America: Elsevier Science Inc., 660 White Plains Road, Tarrytown, NY 10591-5153, U.S.A.
Rest of the World: Elsevier Science Ltd, The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, U.K.

[Tel. Oxford (01865) 843000; Fax 843969]

Frequency: Published monthly. Copyright © 1995 Elsevier Science Ltd

Subscription Rates

Annual institutional subscription rate (1996): North, Central and South America, US\$1174.00, Rest of World, £738.00. Associated Personal Subscription Rates are available on request for those whose institutions are library subscribers. Sterling prices exclude VAT. Non-VAT registered customers in the European Community will be charged the appropriate VAT in addition to the price listed. Prices include postage and insurance and are subject to change without notice.

Back Issues

Back issues of all previously published volumes are available direct from Elsevier Science Offices (Oxford and New York). Complete volumes and single issues can be purchased for 1991-95. Earlier issues are available in high quality photo-duplicated copies as complete volumes only.

Second class postage paid at NEWARK NJ. Postmaster send address corrections to *Computers & Chemical Engineering*, c/o Elsevier Science Inc., 660 White Plains Road, Tarrytown, NY 10591-5153, U.S.A.

LIST OF CONTENTS

NUMBER 1

T. A. Badgwell, T. Breedijk,
S. G. Bushman, S. W. Butler,
S. Chatterjee, T. F. Edgar,
A. J. Toprac and I. Trachtenberg

P. L. Spedding and R. M. Spencer 43 Simulation of packing density and liquid flow in fixed beds

A. K. Modi, A. Newell,
D. M. Steier and A. W. Westerberg 75 Building a chemical process design system within Soar—I. Design issues

F. Ercal, N. L. Book, S. Pait and J. J. Fielding 91 An efficient multicomputer algorithm for the solution of chemical process flowsheeting equations

H. W. Andersen, L. Laroche and M. Morari 105 Effect of design on the operation of homogeneous azeotropic distillation

Short Note

R. Carta, G. Tola, A. Servida and M. Morbidelli 123 Error analysis of collocation models for steady-state multistage separation units

NUMBER 2

R. S. H. Mah, A. C. Tamhane, S. H. Tung and A. N. Patel 129 Process trending with piecewise linear smoothing

J. J. Romainainen and T. Salmi 139 Numerical strategies in solving gas-liquid reactor models—3. Steady state bubble columns

P. Terwiesch and M. Agarwal 155 A discretized nonlinear state estimator for batch processes

L. Megan and D. J. Cooper 171 A neural network strategy for disturbance pattern classification and adaptive multivariable control

J. Zhou and R. H. Luecke 187 Estimation of the covariances of the process noise and measurement noise for a linear discrete dynamic system

X. X. Zhu, B. K. O'Neill, J. R. Roach and R. M. Wood 197 A new method for heat exchanger network synthesis using area targeting procedures

X. X. Zhu, B. K. O'Neill, J. R. Roach and R. M. Wood 223 Area-targeting methods for the direct synthesis of heat exchanger networks with unequal film coefficients

A. Abbas and P. E. Sawyer 241 A multiobjective design algorithm: application to the design of SISO control systems

*Short Note***M. Chidambaram and G. P. Reddy**

249

Nonlinear control of systems with input multiplicities

NUMBER 3

O. R. Boissel and J. C. Kantor 253 Optimal feedback control design for discrete-event systems using simulated annealing

R. Bañares-Alcántara 267 Design support systems for process engineering—I. Requirements and proposed solutions for a design process representation

R. Bañares-Alcántara and H. M. S. Lababidi 279 Design support systems for process engineering—II. KBDS: an experimental prototype

O. Taiwo, J. Schultz and V. Krebs 303 A comparison of two methods for the numerical inversion of Laplace transforms

W. Prager and G. Propst 309 A dynamic two-phase flow model for a purification plant

P. R. Lyman and C. Georgakis 321 Plant-wide control of the Tennessee Eastman problem

L. M. Ribeiro, P. F. R. Regueiras, M. M. L. Guimarães, C. M. N. Madureira and J. J. C. Cruz-Pinto 333 The dynamic behaviour of liquid–liquid agitated dispersions—I. The hydrodynamics

A. K. Modi, A. Newell, D. M. Steier and A. W. Westerberg 345 Building a chemical process design system with Soar—2. Learning issues

Gh. Juncu and O. Floarea 363 Multiplicity analysis of the 2-D model of the catalytic porous wall reactor with axial flow

NUMBER 4

D. Tieu, W. R. Cluett and A. Penlidis 375 A comparison of collocation methods for solving dynamic optimization problems

A. A. Adetayo, J. D. Litster and I. T. Cameron 383 Steady state modelling and simulation of a fertilizer granulation circuit

G. Buzad and M. F. Doherty 395 New tools for the design of kinetically controlled reactive distillation columns for ternary mixtures

P. Lundström, J. H. Lee, M. Morari and S. Skogestad 409 Limitations of dynamic matrix control

T. Ajzoul, C. Chaussavoine and M. Amouroux 423 Finite element analysis of a transient nonlinear heat transfer problem

A. N. Sathyagal, D. Ramkrishna and G. Narsimhan	437	Solution of inverse problems in population balances—II. Particle break-up
A. Banerjee and Y. Arkun	453	Control configuration design applied to the Tennessee Eastman plant-wide control problem
L. O. A. Maia, L. A. Vidal de Carvalho and R. Y. Qassim	481	Synthesis of utility systems by simulated annealing
<i>Short Notes</i>		
V. G. Dovi	489	Use of slack variables in the mathematical modelling of reaction equilibria in complex chemical kinetics
E. Eckert and M. Kubíček	493	Bubble and dew point calculation for multiple liquid cases
<i>Erratum</i>	495	
NUMBER 5		
D. K. Varvarigos, L. T. Biegler and I. E. Grossmann	497	Modeling uncertainty and analyzing bottleneck characteristics in multiperiod design optimization
S. A. Dadebo and K. B. McAuley	513	Dynamic optimization of constrained chemical engineering problems using dynamic programming
J. Y. Choi, H. G. Pandit, R. R. Rhinehart and R. J. Farrell	527	A process simulator for pH control studies
J. B. Riggs, K. Curtner and W. Foslien	541	Comparison of two advanced steam temperature controllers for coal-fired boilers
H. S. Ryoo and N. V. Sahinidis	551	Global optimization of nonconvex NLPs and MINLPs with applications in process design
L. S. Jennings, K. L. Teo, F. Y. Wang and Q. Yu	567	Optimal protein separation
N. M. Iyer and A. E. Farrell	575	Adaptive input-output linearizing control of a continuous stirred tank reactor
C. T. Kiranoudis, Z. B. Maroulis and D. Marinou-Kouris	581	Design and production planning for multiproduct dehydration plants
<i>Short Notes</i>		
K. M. Hangos and E. I. Varga	607	Note on the effect of recycle on the dynamics of chemical process plants
J. Kuck	611	A non-iterative algorithm for a catalyst model

NUMBER 6/7

APPLICATIONS OF PARALLEL COMPUTING

Guest Editorial

Antony N. Beris and **Donald L. Miller** v

APPLICATIONS TO TRANSPORT PHENOMENA AND REACTION ENGINEERING

S. Chen, S. P. Dawson, G. D. Doolen, 617 Lattice methods and their applications to reacting systems

D. R. Janecky and A. Lawmiezak

R. Keunings 647 Parallel finite element algorithms applied to computational rheology

N. K. Ingle and T. J. Mountziaris 671 A multifrontal algorithm for the solution of large systems of equations using network-based parallel computing

H. Yang and S. Kim 683 Boundary element analysis of particle mobilities in a cylindrical channel: network-based parallel computing with Condor

S. R. Rastogi and N. J. Wagner 693 Massively parallel non-equilibrium Brownian dynamics simulations for complex fluids: the rheology of Brownian suspensions

S. M. Stark, M. Neurock and **M. T. Klein** 719 Comparison of MIMD and SIMD strategies for Monte Carlo modelling of kinetically coupled reactions

F. Traenkle, M. D. Hill and **S. Kim** 743 Solving microstructure electrostatics on a proposed parallel computer

APPLICATIONS TO PROCESS DESIGN, SYNTHESIS AND OPTIMIZATION

E. S. Fraga and K. I. M. McKinnon 759 Portable code for process synthesis using workstation clusters and distributed memory multicompilers

J. E. Killough 775 The application of parallel computing to the flow of fluids in porous media

A. B. Coon and M. A. Stadtherr 787 Generalized block-tridiagonal matrix orderings for parallel computation in process flowsheeting

K. A. High and R. D. LaRoche 807 Parallel nonlinear optimization techniques for chemical process design problems

I. P. Androulakis and G. V. Reklaitis 827 Analysis of the spurious behavior of asynchronous relaxation algorithms

G. K. Kudva and J. F. Pekny 847 DCABB: a distributed control architecture for branch and bound calculations

Announcement I

NUMBER 8

**J. Unger, A. Kröner
and W. Marquardt** 867 Structural analysis of Differential-Algebraic Equation systems—theory and applications

B. Lee and G. V. Reklaitis 883 Optimal scheduling of cyclic batch processes for heat integration—I. Basic formulation

B. Lee and G. V. Reklaitis 907 Optimal scheduling of cyclic batch processes for heat integration—II. Extended problems

R. S. Kanadibhotla and J. B. Riggs 933 Nonlinear model based control of a recycle reactor process

NUMBER 9

N. L. Ricker 949 Optimal steady-state operation of the Tennessee Eastman Challenge Process

N. L. Ricker and J. H. Lee 961 Nonlinear model predictive control of the Tennessee Eastman Challenge Process

N. L. Ricker and J. H. Lee 983 Nonlinear modeling and state estimation for the Tennessee Eastman Challenge Process

N. Aguilera and G. Nasini 1007 Flexibility test for heat exchanger networks with uncertain flowrates

M. Caracotsios and W. E. Stewart 1019 Sensitivity analysis of initial-boundary-value problems with mixed PDEs and algebraic equations. Applications to chemical and biochemical systems

NUMBER 10

**J. S. Albuquerque
and L. T. Biegler** 1031 Decomposition algorithms for on-line estimation with nonlinear models

S. Viacoumi and C. Tien 1041 Uptake of organic compounds from aqueous solutions by soils—a comparison of two Laplace transform inversion techniques

**R. M. Enick, S. M. Klara
and J. J. Marano** 1051 A robust algorithm for high-pressure gas humidification

Gh. Juncu and O. Floarea 1063 Multiplicity pattern in the nonisothermal nonadiabatic packed bed chemical reactor

**M. Tandon, P. T. Cummings
and M. D. LeVan** 1069 Scheduling of multiple products on parallel units with tardiness penalties using simulated annealing

**J. C. MacMurray
and D. M. Himmelblau** 1077 Modeling and control of a packed distillation column using artificial neural networks

**E. N. Pistikopoulos
and M. G. Ierapetritou** 1089 Novel approach for optimal process design under uncertainty

Announcement

I

NUMBER 11

G. V. Reklaitis iii Announcement—Best Paper of 1992

**C. M. McDonald
and C. A. Floudas** 1111 Global optimization for the phase and chemical equilibrium problem: Application to the NRTL equation

**R. Carta, G. Tola, A. Servida
and M. Morbidelli** 1141 Performance of collocation models for simulating transient multistage separation units

**P. D. Khandalekar
and J. B. Riggs** 1153 Nonlinear process model based control and optimization of a model IV FCC unit

**A. Spence, D. J. Worth
and S. T. Kolaczkowski** 1169 The treatment of non-integer exponents in reaction rate expressions

C. L. E. Swartz 1173 An algorithm for hierarchical supervisory control

**S. D. Dimitrov
and D. I. Kamenski** 1181 A parameter estimation method for systems of rational functions

Y. Qian and K. M. Lien 1185 Rule based synthesis of separation systems by predictive best first search with rules represented as trapezoidal numbers

B. Rosendall and B. A. Finlayson 1207 Transport effects in packed-bed oxidation reactors

NUMBER 12

I. Quesada and I. E. Grossmann 1219 Global optimization of bilinear process networks with multicomponent flows

J. R. Paloschi 1243 Bounded homotopies to solve systems of algebraic nonlinear equations

A. Kovač and P. Glavić 1255 Retrofit of complex and energy intensive processes—I

M. Guay and D. D. McLean 1271 Optimization and sensitivity analysis for multi-response parameter estimation in systems of ordinary differential equations

**J. L. Harmon, Ph. Duboc
and D. Bonvin** 1287 Factor analytical modeling of biochemical data

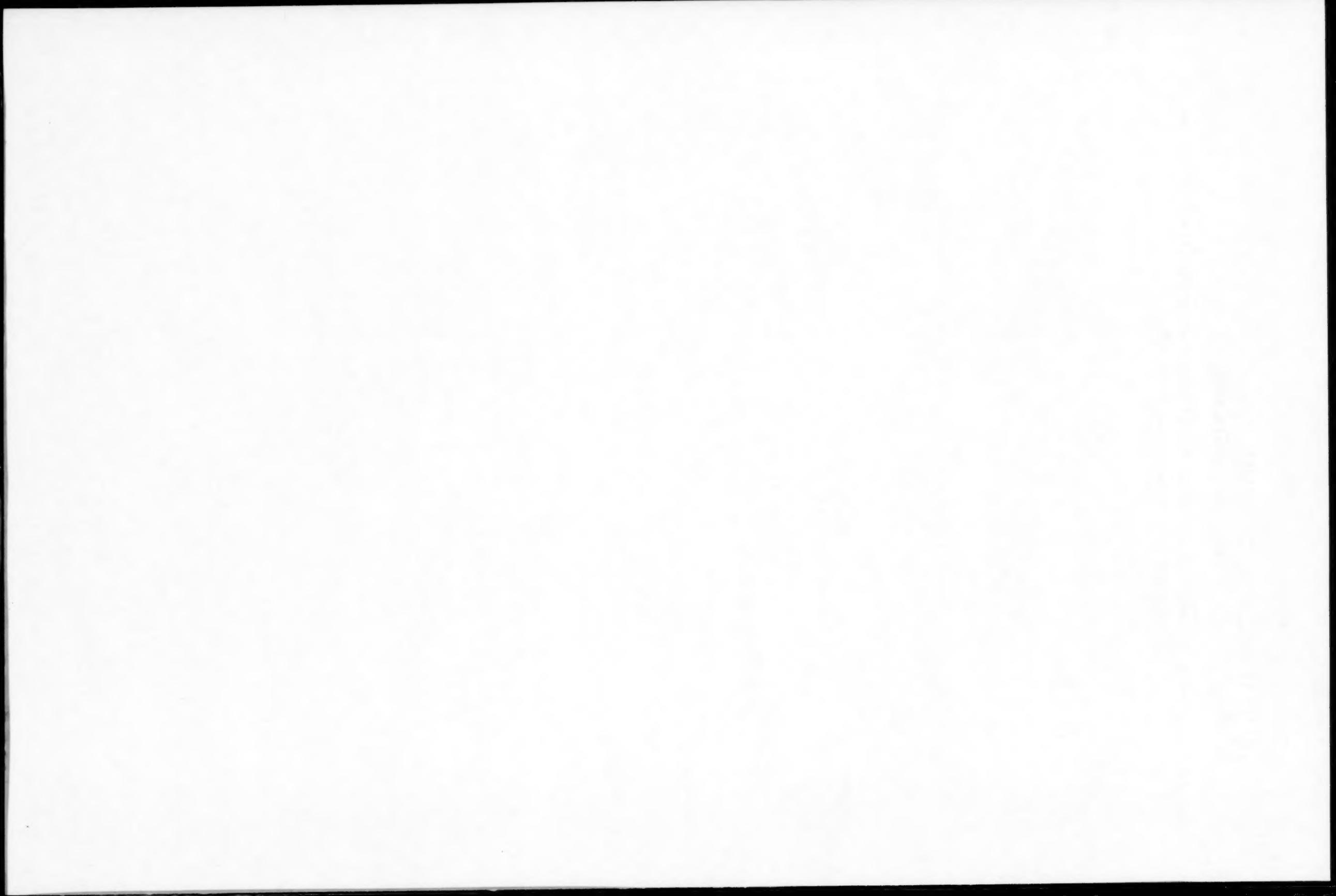
**D. K. Varvarezos, I. E. Grossmann
and L. T. Biegler** 1301 A sensitivity based approach for flexibility analysis and design of linear process systems

Contents

ix

VOL. 19 SUPPLEMENT

ESCAPE-5 (European Symposium on Computer Aided Process Engineering—5) was produced as a Supplement to the journal during 1995.



AUTHOR INDEX

Abbas A., 241
 Adetayo A. A., 383
 Agarwal M., 155
 Aguilera N., 1007
 Ajzoul T., 423
 Albuquerque J. S., 1031
 Amouroux M., 423
 Andersen H. W., 105
 Androulakis I. P., 827
 Arkun Y., 453
 Badgwell T. A., 1
 Bañares-Alcántara R., 267, 279
 Banerjee A., 453
 Beris A. N., v
 Biegler L. T., 497, 1031, 1301
 Boissel O. R., 253
 Bonvin D., 1287
 Book N. L., 91
 Breedijk T., 1
 Bushman S. G., 1
 Butler S. W., 1
 Buzad G., 395
 Cameron I. T., 383
 Caracotsios M., 1019
 Carta R., 123, 1141
 Chatterjee S., 1
 Chaussovoine C., 423
 Chen S., 647
 Chidambaram M., 249
 Choi J. Y., 527
 Cluett W. R., 375
 Coon A. B., 787
 Cooper D. J., 171
 Cruz-Pinto J. J. C., 333
 Cummings P. T., 1069
 Curtner K., 541
 Dadebo S. A., 513
 Dawson S. P., 647
 Dimitrov S., 1181
 Doherty M. F., 395
 Doolen G. D., 647
 Dovi V. G., 489
 Duboc Ph., 1287
 Eckert E., 493
 Edgar T. F., 1
 Enick R. M., 1051
 Ercal F., 91
 Farrell A. E., 575
 Farrell R. J., 527
 Fielding J. J., 91
 Finlayson B. A., 1207
 Floarea O., 363, 1063
 Floudas C. A., 1111
 Foslien W., 541
 Fraga E. S., 775
 Georgakis C., 321
 Glavić P., 1255
 Grossmann I. E., 497, 1219, 1301
 Guay M., 1271
 Guimaraes M. M. L., 333
 Hangos K. M., 607
 Harmon J. L., 1287
 High K. A., 807
 Hill M. D., 759
 Himmelblau D. M., 1077
 Ierapetritou M. G., 1089
 Ingle N. K., 683
 Iyer N. M., 575
 Janecky D. R., 647
 Jennings L. S., 567
 Juncu Gh., 363, 1063
 Kamenski D. I., 1181
 Kanadibhotla R. S., 933
 Kantor J. C., 253
 Keunings R., 671
 Khandalekar P. D., 1153
 Killough J. E., 775
 Kim S., 693, 759
 Kiranoudis C. T., 581
 Klara S. M., 1051
 Klein M. T., 743
 Kolaczkowski S. T., 1169
 Kováč A., 1255
 Krebs V., 303
 Kröner A., 867
 Kubíček M., 493
 Kuck J., 611
 Kudva G. K., 847
 LaRoche R. D., 807
 Lababidi H. M. S., 279
 Laroche L., 105
 Lawniczak A., 647
 LeVan M. D., 1069
 Lee B., 883, 907
 Lee J. H., 409, 961, 983
 Lien K. M., 1185
 Lister J. D., 383
 Luecke R. H., 187
 Lundström P., 409
 Lyman P. R., 321
 MacMurray J. C., 1077
 Madureira C. M. N., 333
 Mah R. S. H., 129
 Maia L. O. A., 481
 Marano J. J., 1051
 Marinatos-Kouris D., 581
 Maroulis Z. B., 581
 Marquardt W., 867
 McAvooy T. J., 495
 McDonald C. M., 1111
 McKinnon K. I. M., 775
 McLean D. D., 1271
 Mcaulley K. B., 513
 Megan L., 171
 Miller D. L., v
 Modi A. K., 75, 345
 Morari M., 105, 409
 Morbidelli M., 123, 1141
 Mountzaris T. J., 683
 Narsimhan G., 437
 Nasini G., 1007
 Neurock M., 743
 Newell A., 75, 345
 O'Neill B. K., 197, 223
 Pait S., 91
 Paloschi J. R., 1243
 Pandit H. G., 527
 Patel A. N., 129
 Pekny J. F., 847
 Penlidis A., 375
 Pistikopoulos E. N., 1089
 Prager W., 309
 Propst G., 309
 Qassim R. Y., 481
 Qian Y., 1185
 Quesada I., 1219
 Ramkrishna D., 437
 Rastogi S. R., 719
 Reddy G. P., 249
 Regueiras P. F. R., 333
 Reklaitis G. V., iii, 827, 883, 907
 Rhinehart R. R., 527
 Ribeiro L. M., 333
 Ricker N. L., 949, 961, 983
 Riggs J. B., 541, 933, 1153
 Roach J. R., 197, 223
 Romanainen J. J., 139
 Rosendall B., 1207
 Ryoo H. S., 551
 Sahinidis N. V., 551
 Salmi T., 139
 Sathyagal A. N., 437
 Sawyer P. E., 241
 Schultz J., 303
 Servida A., 123, 1141
 Skogestad S., 409
 Spedding P. L., 43
 Spence A., 1169
 Spencer R. M., 43
 Stadherr M. A., 787
 Stark S. M., 743
 Steier D. M., 75, 345
 Stewart W. E., 1019
 Swartz C. L. E., 1173
 Taiwo O., 303
 Tamhane A. C., 129
 Tandon M., 1069
 Teo K. L., 567
 Terwiesch P., 155
 Tien C., 1041
 Tieu D., 375
 Tola G., 123, 1141
 Toprac A. J., 1
 Trachtenberg I., 1

Traenkle F., 759
Tung S. H., 129
Unger J., 867
Varga E. I., 607
Varvarezos D. K., 497, 1301

Vidal de Carvalho L. A., 481
Wagner N. J., 719
Wang F. Y., 567
Westerberg A. W., 75, 345
Wood R. M., 197, 223
Worth D. J., 1169

Yang H., 693
Ye N., 495
Yiacoumi S., 1041
Yu Q., 567
Zhou J., 187
Zhu X. X., 197, 223